STN Columbus

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      3
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                 information from the epoline Register
         JUL 28
                 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
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                 STN Viewer performance improved
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                 CA/CAplus enhanced with printed Chemical Abstracts
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                 Multiple databases enhanced for more flexible patent
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                 Current-awareness alert (SDI) setup and editing
                 enhanced
         OCT 22
                 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
NEWS 20
                 Applications
NEWS 21
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                 CHEMLIST enhanced with intermediate list of
                 pre-registered REACH substances
NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
             AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS LOGIN
              Welcome Banner and News Items
              For general information regarding STN implementation of IPC 8
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FILE 'HOME' ENTERED AT 00:36:50 ON 19 NOV 2008
=> file reg
                                                SINCE FILE
                                                                TOTAL
COST IN U.S. DOLLARS
                                                     ENTRY
                                                              SESSION
FULL ESTIMATED COST
                                                      0.21
                                                                 0.21
```

FILE 'REGISTRY' ENTERED AT 00:37:14 ON 19 NOV 2008

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```
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```

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STRUCTURE FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9 DICTIONARY FILE UPDATES: 17 NOV 2008 HIGHEST RN 1073055-74-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> e abacavir/cn
                  ABACA/CN
            1
             1
E2
                  ABACA MANILA HEMP/CN
             1 --> ABACAVIR/CN
E.3
                 ABACAVIR 5'-MONOPHOSPHATE DEAMINASE/CN
E4
             1
E5
                  ABACAVIR MONOPHOSPHATE DEAMINASE/CN
                 ABACAVIR SUCCINATE/CN
Ε6
             1
                 ABACAVIR SULFATE/CN
E7
            1
                 ABACAVIR SULFATE-LAMIVUDINE MIXT./CN
Ε8
            1
E9
            1
                 ABACAVIR-EPIVIR MIXT./CN
                 ABACIL/CN
E10
            1
                  ABACIN/CN
            1
E11
E12
             1
                  ABACOPTERIN A/CN
=> s e3
             1 ABACAVIR/CN
L1
=> d
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
1.1
     136470-78-5 REGISTRY
     Entered STN: 04 Oct 1991
ED
     2-Cyclopentene-1-methanol, 4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-
CN
     , (1S, 4R) - (CA INDEX NAME)
OTHER CA INDEX NAMES:
    2-Cyclopentene-1-methanol, 4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-
     , (1S-cis)-
OTHER NAMES:
CN
    1592U89
CN
    Abacavir
CN
    Ziagen
FS
     STEREOSEARCH
MF
    C14 H18 N6 O
CI
    COM
SR
     CA
LC
                 ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO,
     STN Files:
       CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU, EMBASE,
       IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MRCK*, PATDPASPC,
       PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:
                     WHO
```

Absolute stereochemistry. Rotation (-).

```
NH.
                      Ν.,
                                                   OΗ
HoN
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1298 REFERENCES IN FILE CA (1907 TO DATE) 16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 1305 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 7.61 7.82

FULL ESTIMATED COST

FILE 'MRCK' ENTERED AT 00:37:44 ON 19 NOV 2008 COPYRIGHT (C) 2008 Merck & Co., Inc., Whitehouse Station, New Jersey, USA. All Rights Reserve

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=> s 11

L21 L1

=> d all

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(MNO): 1400001 MERCK Number

CAS Registry No. (RN): 136470-78-5

MERCK Index Name (MIN): Abacavir

(CN): (1S, 4R) - 4 - [2-Amino-6 - (cyclopropylamino) - 9H-purin - 9-y1] -CA Index Name

2-cyclopentene-1-methanol

Synonym(s) (CN): (-)-cis-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-

2-cyclopentene-1-methanol

Drug Code(s) (CN): 1592U89

(FS): Active Monographs File Segment.

Molecular Form. (MF): C14 H18 N6 O

Wgt Composition (COMP): C 58.73%, H 6.34%, N 29.35%, O 5.59%.

Molecular Weight (MW): 286.33

References (RE): Nucleoside reverse transcriptase inhibitor (NRTI). S. M. Daluge, EP 349242 (1990 to Wellcome Found.); idem, US 5034394 (1991 to Burroughs Wellcome). Asymmetric synthesis: M. T. Crimmins, B. W. King, J. Org. Chem. 61, 4192 (1996). Pharmacology and biological profile: S. M. Daluge et al., Antimicrob. Agents Chemother. 41, 1082 (1997). Review of antiviral activity and clinical evaluations: R. H. Foster, D. Faulds, Drugs 55, 729-736 (1998). Clinical trial of triple nucleoside regimen in HIV patients: S. Staszewski et al., J. Am.

Med. Assoc. 285, 1155 (2001).

Absolute stereochemistry. Rotation (-).

```
Melting Point (MP):
```

Value MP deg C ===== 165

Optical Rotatory Power (ORP):

UV Spectrum (UVS):

Other Properties (OCPP):

CM

1

White solid foam from acetonitrile, mp 165°. uv max (pH 1): 296 , 255 nm (\$\epsilon\$ 14000, 10700) ; uv max (pH 7): 284 , 259 nm (\$\epsilon\$ 15900, 9200) ; uv max (pH 13): 284 , 259 nm (\$\epsilon\$ 15800, 9100) . [\$\alpha\$] D20 -59.7° ; [\$\alpha\$] 43620 -127.8° ; [\$\alpha\$] 36520 -218.1° (c = 0.15 in methanol) . Log P (1-octanol/0.1M sodium phosphate): 1.22 \$\pmu\$0.03 (pH 7.4). pKa 5.01. Soly in water (25°): >80 mM (pH 7).

```
== DERIVATIVE == (1): Sulfate
CAS Registry No. (RN.DRV): 188062-50-2
Trade Name(s) (CN.DRV): Ziagen (GlaxoSmithKline plc; GSK)
Molecular Form. (MF.DRV): (C14 H18 N6 O)2 . H2 O4 S
Wgt Composition (COMP.DRV): C 50.14%, H 5.71%, N 25.06%, O 14.31%, S 4.78%.
Molecular Weight (MW.DRV): 670.74
```

Absolute stereochemistry. Rotation (-).

CM 2

Therapeutic Codes (THER):
 Antiretroviral.
Referenced Patent (RPN):
 EP349242; US5034394

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL SESSION 4.11 11.93

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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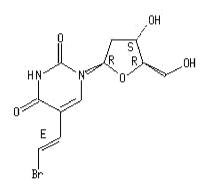
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> e	brivudine/cn	
E1	1	BRIVIOLIDE J/CN
E2	1	BRIVUDIN/CN
E3	1>	BRIVUDINE/CN
E4	1	BRIX (HUMAN CLONE MGC:45062 IMAGE:5107954)/CN
E5	1	BRIX (HUMAN CLONE MGC:4924 IMAGE:3462041 GENE BRIX)/CN
E6	1	BRIX (XENOPUS LAEVIS GENE BRIX)/CN
E7	1	BRIX DOMAIN CONTAINING 1 (HUMAN CLONE MGC:21067 IMAGE:474552
		4 GENE BXDC1)/CN
E8	1	BRIX DOMAIN CONTAINING 1 (HUMAN CLONE MGC:21067 IMAGE:474552
		4)/CN
E9	1	BRIX DOMAIN CONTAINING 1 (MOUSE STRAIN CZECH II CLONE MGC:35

```
797 IMAGE: 4009314)/CN
E10
                      BRIX DOMAIN CONTAINING-LIKE PROTEIN (LEISHMANIA MAJOR STRAIN
E11
               1
                      BRIX DOMAIN PROTEIN (SULFOLOBUS ACIDOCALDARIUS STRAIN DSM 63
                      9)/CN
                      BRIX-DOMAIN RIBOSOMAL BIOGENESIS PROTEIN (METHANOBREVIBACTER
E12
                       SMITHII STRAIN ATCC 35061)/CN
=> s e3
               1 BRIVUDINE/CN
L3
=> d
L3
      ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
      69304-47-8 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Uridine, 5-[(1E)-2-bromoethenyl]-2'-deoxy- (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Uridine, 5-(2-bromoethenyl)-2'-deoxy-, (E)-
CN
OTHER NAMES:
      (E)-5-(2-Bromovinyl)-2'-deoxyuridine
CN
      (E)-5-(2-Bromovinyl) deoxyuridine
CN
CN
      (E)-5-0-(2-bromoethenyl)-2'-deoxyuridine
      5-[(E)-2-Bromoethenyl]-2'-deoxyuridine
CN
CN
      Brivudin
     Brivudine
CN
      Bromovinyldeoxyuridine
CN
CN
      BVDU
CN
      Helpin
      STEREOSEARCH
FS
      102040-00-6, 155203-57-9, 286419-83-8
DR
      C11 H13 Br N2 O5
MF
CI
      STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CIN, CSCHEM,
LC
        DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
           (*File contains numerically searchable property data)
      Other Sources:
```

Absolute stereochemistry. Double bond geometry as shown.



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
```

576 REFERENCES IN FILE CA (1907 TO DATE)
27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
579 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file reg
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
7.61
19.54

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http://www.cas.org/support/stngen/stndoc/properties.html

```
=> e cidofovir/cn
E.1
             1
                   CIDIROL/CN
E2
             1
                   CIDOCETINE/CN
             1 --> CIDOFOVIR/CN
E3
                  CIDOFOVIR DIPHOSPHATE/CN
E4
             1
E5
             1
                  CIDOFOVIR HYDRATE/CN
             1
                  CIDOMYCIN/CN
E6
E7
             1
                  CIDOPHAGE/CN
                  CIDOPHYLLINE/CN
E.8
             1
E9
             1
                  CIDOTEN/CN
E10
             1
                  CIDOVIR/CN
E11
            1
                  CIDOXEPIN/CN
E12
             1
                  CIDOXEPIN HYDROCHLORIDE/CN
=> s e3
             1 CIDOFOVIR/CN
L4
=> d
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
T. 4
     113852-37-2 REGISTRY
RN
ED
     Entered STN: 16 Apr 1988
     Phosphonic acid, P-[[(1S)-2-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-
CN
     (hydroxymethyl)ethoxy]methyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Phosphonic acid, [(1S)-2-(4-amino-2-oxo-1(2H)-pyrimidiny1)-1-
     (hydroxymethyl)ethoxy]methyl]- (9CI)
     Phosphonic acid, [[2-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-
CN
     (hydroxymethyl)ethoxy]methyl]-, (S)-
OTHER NAMES:
CN
     (S)-1-(3-hydroxy-2-phosphonomethoxypropyl) cytosine
     (S)-HPMPC
CN
     1-(S)-(3-Hydroxy-2-phosphonylmethoxypropyl)cytosine
CN
     1-[(S)-3-Hydroxy-2-(phosphonomethoxy)propyl]cytosine
CN
CN
     Cidofovir
CN
     Cidovir
CN
     GS 0504
CN
     HPMPC
CN
     Vistide
FS
     STEREOSEARCH
MF
     C8 H14 N3 O6 P
     COM
CI
SR
                  ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS,
LC
     STN Files:
       BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST,
       CIN, DDFU, DRUGU, EMBASE, HSDB*, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS,
```

IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, PATDPASPC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU

(*File contains numerically searchable property data)

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

836 REFERENCES IN FILE CA (1907 TO DATE)

36 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

840 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file merck COST IN U.S. DOLLARS

SINCE FILE TOTAL. ENTRY SESSION 7.61 27.15

FULL ESTIMATED COST

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=> s 14

L5 1 L4

=> d all

ANSWER 1 OF 1 MRCK COPYRIGHT (C) 2008 Merck and Co., Inc., L5

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MERCK Number

(MNO): 1402268 (RN): **113852-37-2** CAS Registry No.

MERCK Index Name (MIN): Cidofovir

CA Index Name (CN): [[(1S)-2-(4-Amino-2-oxo-1(2H)-pyrimidinyl)-1-

(hydroxymethyl)ethoxy]methyl]phosphonic acid

Synonym(s) (CN): (S)-1-[3-hydroxy-2-(phosphonylmethoxy)propyl]cytosine;

(S)-HPMPC

Drug Code(s) (CN): GS-504

Trade Name(s) (CN): Vistide (Gilead Sciences; Gilead)

(FS): Active Monographs File Segment.

Molecular Form. (MF): C8 H14 N3 O6 P

Wqt Composition (COMP): C 34.42%, H 5.05%, N 15.05%, O 34.38%, P 11.09%.

Molecular Weight (MW): 279.19

(RE): DNA synthesis inhibitor. Prepn: A. Holy et al., EP References 253412; eidem, US 5142051 (1988, 1992 both to Ceskoslov. Akad. Ved; Rega Inst.); and activity vs cytomegalovirus: R. Snoeck et al., Antimicrob. Agents Chemother. 32, 1839 (1988). Syntheses: J. J. Bronson et al., Nucleosides Nucleotides 9, 745 (1990); P. R. Brodfuehrer et al., Tetrahedron Lett. 35, 3243 (1994). Activity vs herpes simplex virus: G. Andrei et al., Eur. J. Clin. Microbiol. Infect. Dis. 11, 143 (1992). Review of pharmacology and clinical studies: M. J. M. Hitchcock et al., Antivir. Chem. Chemother. 7, 115-127 (1996). Review of clinical potential in poxvirus infections: E. De Clercq, Trends Pharmacol. Sci. 23, 456-458

Absolute stereochemistry.

```
Melting Point (MP):
Value|
MP |Note
deg C|
____+__
 260 | (dec)
Optical Rotatory Power (ORP):
         |Spectral|
Value|Temp.| Line
 ORP | ORP.T| ORP.SL
                           Note
 deg |deg C|
-97.3 \mid 20 \mid D \mid (c = 0.80 \text{ in water})
UV Spectrum (UVS):
Maximum |
Peak Pos. |
 UVS.PP |
                   Note
  nm
279 | (pH 2) (\epsilon 13000)
Other Properties (OCPP):
    Fluffy white powder, mp 260° (dec) . [\alpha]D20 -97.3° (c = 0.80 in water) . Monohydrate, uv max (pH 2): 279 nm (\epsilon
     13000) .
Therapeutic Codes (THER):
     Antiviral.
Referenced Patent (RPN):
    EP253412; US5142051
=> log y
                                                 SINCE FILE
                                                                 TOTAL
COST IN U.S. DOLLARS
                                                      ENTRY
                                                               SESSION
```

2.79

29.94

STN INTERNATIONAL LOGOFF AT 00:40:13 ON 19 NOV 2008

FULL ESTIMATED COST